



chain nodes :

7 8 14 15 17 18 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41
42 43 44 45 46 47 48 55 56 63 64 83 84 102 103 121 122 129

ring nodes :

1 2 3 4 5 6 9 10 11 12 13 19 20 21 22 23 24 49 50 51 52 53 54 57
58 59 60 61 62 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81
82 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 104 105 106
107 108 109 110 111 112 113 114 115 116 117 118 119 120

chain bonds :

1-9 4-7 5-18 6-8 10-17 12-14 14-15 18-129 20-26 24-25 25-27 26-28 27-29
27-30 28-31 28-32 29-33 30-34 31-35 32-36 33-43 33-44 34-41 34-42 35-37 35-39
36-38 36-40 39-47 40-48 42-46 44-45 49-55 55-56 56-60 58-64 62-63 66-83 70-72
76-78 82-84 86-102 90-98 92-101 96-103 105-121 109-117 111-120 115-122

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-13 10-11 11-12 12-13 19-20 19-24 20-21 21-22
22-23 23-24 49-50 49-54 50-51 51-52 52-53 53-54 57-58 57-62 58-59 59-60 60-61
61-62 65-66 65-70 66-67 67-68 68-69 69-70 71-72 71-76 72-73 73-74 74-75 75-76
77-78 77-82 78-79 79-80 80-81 81-82 85-86 85-90 86-87 87-88 88-89 89-90 91-92
91-96 92-93 93-94 94-95 95-96 97-98 97-101 98-99 99-100 100-101 104-105
104-109 105-106 106-107 107-108 108-109 110-111 110-115 111-112 112-113 113-114
114-115 116-117 116-120 117-118 118-119 119-120

exact/norm bonds :

1-2 1-6 1-9 2-3 3-4 4-5 4-7 5-6 5-18 6-8 9-10 9-13 10-11 10-17 11-12 12-13
14-15 18-129 25-27 26-28 27-29 27-30 28-31 28-32 33-43 33-44 34-41 34-42
35-37 35-39 36-38 36-40 39-47 40-48 42-46 44-45 92-101 97-98 97-101 98-99
99-100 100-101 111-120 116-117 116-120 117-118 118-119 119-120

exact bonds :

12-14 20-26 24-25 29-33 30-34 31-35 32-36 49-55 55-56 56-60 58-64 62-63 66-83
70-72 76-78 82-84 86-102 90-98 96-103 105-121 109-117 115-122

normalized bonds :

19-20 19-24 20-21 21-22 22-23 23-24 49-50 49-54 50-51 51-52 52-53 53-54 57-58
57-62 58-59 59-60 60-61 61-62 65-66 65-70 66-67 67-68 68-69 69-70 71-72 71-76
72-73 73-74 74-75 75-76 77-78 77-82 78-79 79-80 80-81 81-82 85-86 85-90 86-87
87-88 88-89 89-90 91-92 91-96 92-93 93-94 94-95 95-96 104-105 104-109 105-106
106-107

107-108 108-109 110-111 110-115 111-112 112-113 113-114 114-115

G1:H,O,S,N

G2:[*1],[*2],[*3],[*4],[*5]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 17:CLASS 18:CLASS 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS
30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS
39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS
48:CLASS 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:CLASS 56:CLASS
57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:CLASS 64:CLASS 65:Atom
66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom
76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:CLASS 84:CLASS
85:Atom 86:Atom 87:Atom 88:Atom 89:Atom 90:Atom 91:Atom 92:Atom 93:Atom 94:Atom
95:Atom 96:Atom 97:Atom 98:Atom 99:Atom 100:Atom 101:Atom 102:CLASS 103:CLASS
104:Atom 105:Atom 106:Atom 107:Atom 108:Atom 109:Atom 110:Atom 111:Atom 112:Atom
113:Atom 114:Atom 115:Atom 116:Atom 117:Atom 118:Atom 119:Atom 120:Atom 121:CLASS
122:CLASS 129:CLASS